PO1005

Oxidation behavior of superhard Ta-X-C coatings: An ab initio guided approach

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In the sense of environmental sustainability, the application of ultra-stable material systems comes more and more into the focus of academia and industry. Ta-C is one of these highly attractive materials, exhibiting extreme thermal stability (≥ 3000 °C), highest hardness (≥ 40 GPa) and strength, accompanied by strong chemical inertness. Nevertheless, a wide use of Ta-C is intriguingly limited by its unique covalent-metallic bonding character being responsible for the relatively low ductility and strong affinity to oxygen, leading to the formation of partly volatile oxides already in the range of 400 °C (representing $0.1 \cdot T_m$).
Therefore, we applied an ab initio guided approach (Density Functional Theory using VASP) to select alloying elements (X = Zr, Si, Al), which represents the best compromise between increased oxidation resistance, solubility in the preferred face-centred structure, as well as enhanced ductility (fracture toughness). In addition, the influence of carbon vacancies, which can be phase stabilizing in TMCs, is also consider. To verify our theoretical predictions, we deposited the most promising ternary $Ta_{1-y}X_yC$ compounds by non-reactive physical vapour deposition process and oxidized the coatings up to 1600 °C. The kinetic of the oxide scale growth is investigated by HR-TEM, APT, as well as XRD.

Keywords
Ultra-High Temperature Coatings
Ta-X-C
Oxidation Resistance
Super Hardness
DFT